

Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

November 10, 2014

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Pleiades Supercomputer Upgraded with Next-Generation Intel Haswell Processors



- The HECC Supercomputing Systems team upgraded Pleiades with 15 new Haswell compute racks, expanding the supercomputer's capability and increasing its total peak performance by 25% from 3.6 to 4.5 petaflops. There are 72 nodes in each Haswell rack; each node contains 24 cores and 128 GB of RAM.
- HECC engineers integrated the racks into the Pleiades InfiniBand (IB) fabric using a liveintegration method, developed in-house, to minimize the impact on production cycles.
- The integration process was completed in 5 days, well ahead of the planned 13 days, providing more time for early-access users to evaluate the Haswell nodes before they were released into general production (see slide 4).
- A total of 16 Westmere racks were removed in order to accommodate the new racks. These will be kept as spares for the Westmere nodes currently installed in Pleiades and Merope, and may also be incorporated into Merope during a future augmentation.

Mission Impact: To meet NASA's rapidly increasing requirements for high-performance computing, HECC must regularly and significantly upgrade and replace the supercomputing resources it provides to the agency.



The addition of 15 Haswell racks (1080 nodes) increases Pleiades' theoretical peak performance by 25%—from 3.6 to 4.5 petaflops. Each Haswell node delivers 3.34 times the hourly working capacity of a Westmere node.

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'Early Access' Testing Allows Users to Evaluate New Pleiades Hardware & Software



- HECC's Application Performance and Productivity (APP) team initiated a new testing protocol that includes an "early access" period, giving users an opportunity to see how changes affect their application codes and workflows.
- The early access test period was used for the first time with this month's rollout of the new Pleiades SGI racks with Haswell processors (see slide 3).
 - Over 30 users participated, and ran more than 300 jobs during the test. To encourage participation, user accounts were not charged for these jobs.
 - Users were asked to compare different sets of compiler options for building their codes and to report issues. Their results contributed to a new Knowledge Base article, "Preparing to Run on Pleiades Haswell Nodes" (#491).
- HECC teams will continue to use the early access protocol for future hardware/software configuration changes.

Mission Impact: By giving users the ability to perform earlier and more extensive system testing, HECC can reduce risks associated with supercomputing system configuration changes and provide improved documentation that reflects varied user experiences.



Before releasing 15 new Pleiades racks (above) into production, over 30 HECC users ran more than 300 jobs to test application code performance.

POCs: Johnny Chang, johnny.chang@nasa.gov, (650) 604-4356; Robert Hood, robert.hood@nasa.gov, (650) 604-0740; NASA Advanced Supercomputing Division, Computer Sciences Corp.

Upgraded hyperwall in Production After Completion of Software Integration



- HECC's Visualization and Systems teams completed the software integration phase of the hyperwall cluster upgrade. The system is now in production and being utilized for demonstrations.
- The cluster consists of 128 nodes, which are fully integrated into the Pleiades InfiniBand interconnect. Each node has:
 - Two 10-core 2.8-GHz E5-2680v2 Ivy Bridge processors.
 - 64 gigabytes of memory.
 - One NVIDIA GeForce GTX 780 Ti graphics card.
 - Dual FDR (Fourteen Data Rate) InfiniBand cards.
- For the software environment, both teams customized Pleiades' standard systems software for interactive applications. For example:
 - The Systems team implemented security settings that allow hyperwall application software to run across the cluster while following security guidelines.
 - The Visualization team installed software used for demonstrations, such as bigmovie, viewParams, and BigView.
- In addition to running demonstrations, the Visualization team will continue using the hyperwall to perform data analysis on petabyte-scale datasets and to develop high-performance concurrent visualizations.

Mission Impact: The upgraded hyperwall visualization system enables HECC experts, in collaboration with scientific and engineering users, to more effectively visualize and explore the increasingly large datasets produced by NASA supercomputers and instruments.



A 25,600 x 9,600-pixel animation (full hyperwall resolution) showing results of a global simulation at 1/48-degree resolution produced for the Estimating the Circulation and Climate of the Ocean (ECCO) project, displayed on the newly upgraded hyperwall visualization system.

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HECC Engineers Upgrade Router Hardware to Keep Pace with Increased Network Traffic



- HECC Network engineers completed an upgrade of the NAS facility's border and filestaging (aka DMZ) routers to the newest technology from Cisco Systems.
- The new hardware prepares the network for the future by providing 40 and 100-gigabit expansion capability and supports up to 22.8 terabits-per-second of overall network traffic.
- The team also installed new network taps for improved traffic management and security.
- Weeks of careful planning allowed the engineers to complete the transition with minimal impact to users. Remote access to HECC resources was restored after just 20 minutes.
- Since all traffic moving into and out of NASLAN passes through these routers, the added capability of this new hardware is essential to the current and future capacity of the HECC NASLAN environment.

Mission Impact: Improving the capabilities of network routers helps ensure the NASA Advanced Supercomputing (NAS) facility's network capacity will continue to meet the ever-growing demands of the HECC user community.



The new border router (bottom) and network taps (2 grey boxes in the middle) were installed as part of the upgrade to the NASA Advanced Supercomputing facility's network environment.

POCs: Nichole Boscia, nichole.k.boscia@nasa.gov, (650) 604-0891; Harjot Sidhu, harjot.s.sidhu@nasa.gov, (650) 604-4935, NASA Advanced Supercomputing Division, Computer Sciences Corp.

'myNAS' iOS Application for Mobile Job Monitoring Released for Production



- The "myNAS" app for iOS devices is now in production.
 This app provides mobile job monitoring capability for HECC users, enabling them to:
 - View the status of submitted jobs, availability of HECC computing resources, and the latest HECC news.
 - Receive notifications when jobs change state or produce output, even when the app is not running.
 - View text or image output files on their devices (after including a simple command in their job submission script).
- The HECC Application Performance & Productivity, Publications & Media, and Tools teams collaborated to design and develop the myNAS app, a data-gathering agent inside the secure enclave, and a web server that processes and sends the data to the app.
- To ensure proper security, myNAS uses a framework provided by the NASA Center for Internal Mobile Applications. Users must authenticate using their NASA AUID credentials to download and install the app and initiate the first session. Subsequent sessions can be initiated with a PIN.
- A beta version of the app was extensively tested by a subset of HECC users. During testing, some users said they relied on the app's asynchronous notifications of job completions even while logged into the NAS facility's network from their workstations.
- The app is available at https://apps.nasa.gov.

Mission Impact: Providing mobile access to the HECC supercomputing environment improves the productivity of users supporting NASA missions and projects, by enabling them to easily monitor jobs or resource availability from any location with a Wi-Fi or cellular connection.



Information provided by the myNAS app is available via tabs. The Jobs tab (left) shows a user's job list. Selecting a specific job in the list will open the job details view (center); details shown in this view can be customized in the Settings tab. Selecting an output file in the job details view opens the file for viewing (right).

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HECC Technology and Research Showcased During Ames 75th Anniversary Open House



- A team from the HECC Project and the NAS Division coordinated and staffed a highly successful exhibit at the NASA Ames 75th Anniversary Open House on October 18, 2014.
- HECC staff and NAS researchers spent 8 hours interacting with thousands of enthusiastic visitors from across Silicon Valley and the San Francisco Bay Area. Researchers shared their work on large, high-definition screens showing videos of computational fluid dynamics simulations run on the Pleiades supercomputer.
- The NAS exhibit's 8 tents also featured hardware displays including a full-size SGI rack; large posters of visualization images; 18-ft. computer and simulation history timelines; a public-friendly iPadbased interactive quiz (projected onto large monitors); and children's activities.
- Event preparation included extensive planning for displays and exhibits; processing dozens of modeling and simulation videos; creating new computer room "flythrough" and rack component animations; building stands and information placards for hardware displays; creating event signage; and coordinating 37 researchers and event staff.

Mission Impact: Participation in the NASA Ames 75th Anniversary Open House provided an opportunity to convey the importance of NASA missions, showcase the remarkable achievements enabled by HECC resources and technologies, and to engage with students of all ages to spark their enthusiasm for science, math, and technology.



During the NASA Ames open house, researchers discussed their work with enthusiastic participants outside the NAS facility (bottom), some of whom had "backstage passes" enabling them to attend one of seven hyperwall presentations by visualization expert Chris Henze (top).

POC: Gina Morello, gina.f.morello@nasa.gov, (650) 604-4462, NASA Advanced Supercomputing Division

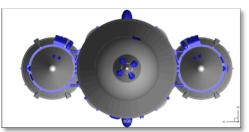
Simulations Run on Pleiades Provide Data for SLS Aerodynamic Database and CDR *

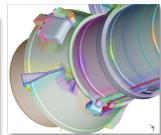


- The NASA Ames Space Launch System (SLS)
 computational fluid dynamics (CFD) team completed
 and delivered extensive ascent aerodynamics
 simulations for the SLS Design Analysis Cycle 3
 (DAC3) vehicle design (SLS-10005). Work included:
 - Using the OVERFLOW CFD code to perform high-fidelity simulations of SLS ascent flow conditions.
 - Simulating 739 ascent cases covering a wide range of Mach numbers and flight angles throughout ascent.
 - Post-processing each case to generate integrated line loads along the vehicle, surface pressures on the SLS and Multi-Purpose Crew Vehicle (MPCV), protuberance air-loads, and vent-location pressure and velocity profiles.
- Cases included a combination of efficient steadystate simulations and time-accurate simulations with unsteady flow.
- Computations were performed using a 375-millionpoint computational grid and required a total of 28 million processor-hours on Pleiades.
- These simulations contribute critical data to the SLS DAC3 Aerodynamic Database being prepared for the upcoming SLS Critical Design Review (CDR).

Mission Impact: High-fidelity computational fluid dynamics simulations of SLS ascent, enabled by the Pleiades supercomputer, provide critical aerodynamic data for trajectory adjustments, structural analyses, and other key studies needed to optimize vehicle safety and performance.







Surface pressures from an OVERFLOW computational fluid dynamics simulation of the Space Launch System Design Analysis Cycle 3 (DAC3) design during ascent (top); model showing protuberance air-load components (lower left); and sample computational grid around a booster nozzle (lower right).

POC: Stuart Rogers, stuart.e.rogers@nasa.gov, (650) 604-4481, NASA Advanced Supercomputing Division

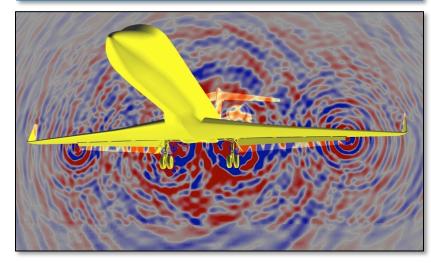
^{*} HECC provided supercomputing resources and services in support of this work

Airframe Noise Visualization Image Featured in *Aviation Week* *



- The September 22nd issue of Aviation Week included an article featuring an image produced by HECC visualization experts, based on computational results from Pleiades.
- "NASA Replans Airframe Noise Work After Gulfstream Withdrawal" describes the greater emphasis that will be placed on simulation methods following the decision by Gulfstream to discontinue flight tests.
- The visualization is based on a mediumresolution gridding of a full aircraft in landing configuration, with the main landing gear and flaps deployed. The dataset was produced using the computational fluid dynamics solver, PowerFLOW, from Exa Corporation.
- Current simulation runs on Pleiades will soon be followed by higher-resolution runs, both with and without noise reduction concepts, in order to identify the most effective noise-reduction strategies.

Mission Impact: Reducing airframe noise is key to enabling commercial aircraft to land at airports with increasingly strict noise regulations. Simulations on Pleiades are playing an important role in the R&D of effective noise reduction concepts.



Visualization of airframe noise sources produced by taking the time derivative of the unsteady pressure field. Red indicates positive regions and blue indicates negative regions. Note the waves that form concentric rings around the outer flap edges, indicating that the edges are relatively strong noise sources. This image appeared in the Sept. 22, 2014 issue of *Aviation Week. Patrick Moran. NASA/Ames*

POCs: Patrick Moran, patrick.moran@nasa.gov, (650) 604-1660, NASA Advanced Supercomputing Division; Mehdi Khorrami, mehdi.r.khorrami@nasa.gov, (757) 864-3630, NASA Langley Research Center

^{*} HECC provided supercomputing resources and services in support of this work

HECC Facility Supported Tours and a Center-Wide Open House in October 2014



- HECC hosted 8 tour groups and one open house in October; guests learned about the agency-wide missions being supported by HECC assets, and viewed the D-Wave Two quantum computer system. Visitors this month included:
 - Chris Clark, mayor of Mountain View, California
 - A group from the Aerospace Safety Advisory Panel visited Ames and were briefed on the Engineering Risk Assessment (ERA) team's results.
 - Astronaut Steven Smith received an overview and tour of the NAS facility.
 - A group from the VTT Technical Research Centre of Finland received an overview and tour of the NAS facility.
 - Associate Administrator Rick Keegan, NASA Mission Support Directorate, received a facility overview, hyperwall demonstration, and a tour of the quantum computer room.
 - 20 Stanford engineering Ph.D. students who visited NASA Ames received a hyperwall demonstration and an overview and tour of the NAS facility, including the main supercomputing room and quantum computing room.
 - At the Ames 75th Anniversary Open House, 7 groups of approximately 30 people each received a 1-hour presentation on the science and engineering accomplishments performed on HECC systems on the new hyperwall. Additionally, thousands of guests were told of the HECC and NAS division accomplishments in 8 tents set up in front of the building.



Chris Clark, mayor of Mountain View, California, poses in front of the D-Wave Two quantum computer during a tour of the NASA Advanced Supercomputing facility. Clark and the Mountain View City Council regularly address issues related to NASA's Ames Research Center.

POC: Gina Morello, gina.f.morello@nasa.gov, (650) 604-4462, NASA Advanced Supercomputing Division

Papers and Presentations



- "Dynamics of Global Atmospheric CO₂ Concentration from 1850 to 2010: A Linear Approximation," W. Wang, R. Nemani, Biogeosciences Discuss., vol. 11, September 29, 2014.
 - http://www.biogeosciences-discuss.net/11/13957/2014/bgd-11-13957-2014.pdf
- "Tidal Disruption and Magnetic Flux Capture: Powering a Jet from a Quiescent Black Hole," L. Z. Kelley, A. Tchekhovskoy, R. Narayan, arXiv:1410.0366 [astro-ph.HE], October 1, 2014. *
 - http://arxiv.org/abs/1410.0366
- "A Global Three Dimensional Radiation Magneto-hydrodynamic Simulation of Super-Eddington Accretion Disks," Y.-F. Jiang, J. M. Stone, S. W. Davis, arXiv:1410.0678 [astro-ph.HE], October 2, 2014. * http://arxiv.org/abs/1410.0678
- "Turbulence-Induced Relative Velocity of Dust Particles IV: the Collision Kernel,"
 L. Pan, P. Padoan, arXiv:1410.1989 [astro-ph.EP], October 8, 2014. *
 http://arxiv.org/abs/1410.1989
- "Electron and Ion Heating by Whistler Turbulence: Three-Dimensional Particle-in-Cell Simulations," R. S. Hughes, S. P. Gary, J. Wang, Los Alamos National Lab repository, for publication in Geophysical Research Letters, October 10, 2014. * http://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-14-27991

^{*} HECC provided supercomputing resources and services in support of this work

Papers and Presentations (cont.)



- "The Origin of Non-Maxwellian Solar Wind Electron Velocity Distribution Function: Connection to Nanoflares in the Solar Corona," H. Che, M. Goldstein, arXiv:1410.4144 [astro-ph.SR], October 15, 2014. * http://arxiv.org/abs/1410.4144
- "Flip-Flop of Oleic Acid in Phospholipid Membrane: Rate and Mechanism," C. Wei, A. Pohorille, The Journal of Physical Chemistry B, October 16, 2014. * http://pubs.acs.org/doi/full/10.1021/jp508163e
- "Kiloparsec-Scale Simulations of Star Formation in Disk Galaxies II. Structure and Dynamics of Filaments and Clumps in Giant Molecular Clouds," M. J. Butler, J. C. Tan, S. Van Loo, arXiv:1410.5541 [astro-ph.SR], October 21, 2014. * http://arxiv.org/abs/1410.5541
- "Numerical Reconstruction of Graphite/Epoxy Composite Microstructure Based on Sub-Micron Resolution X-ray Computing Tomography," M. W. Czabaj, M. L. Riccio, W. W. Whitacre, Composites Science and Technology, October 23, 2014. * http://www.sciencedirect.com/science/article/pii/S0266353814003790
- "Green Leaf Area and Fraction of Photosynthetically Active Radiation Absorbed by Vegetation," S. Ganguly, R. R. Nemani, et al., *Biophysical Applications of Satellite Remote Sensing*, ch. 2, ed. J. Hanes, published in print December 2013, online October 2014. http://books.google.com/books?hl=en&lr=&id=gjW8BAAAQBAJ

^{*} HECC provided supercomputing resources and services in support of this work

Papers and Presentations (cont.)



- "Preface to Solar Dynamics and Magnetism from the Interior to the Atmosphere,"
 N. N. Mansour, A. G. Kosovichev, et al., Solar Dynamics and Magnetism from the Interior to the Atmosphere, eds. N. N. Mansour, A. G. Kosovichev, published in print December 2013, online October 2014.
 - http://books.google.com/books?hl=en&lr=&id=B-29BAAAQBAJ

News and Events

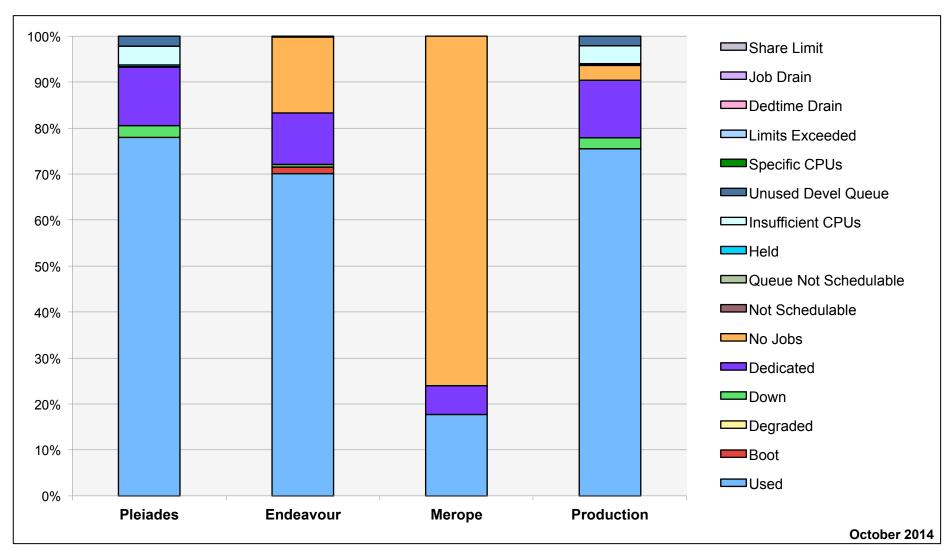


- SC14 Announces New Plenary to Focus on the Importance of Supercomputers in Society, SC14 Blog, September 30, 2014—Supercomputing 2014 announced a new "HPC Matters" plenary led by Dr. Eng Lim Goh, senior vice president and CTO of SGI, featuring NAS Division Chief Piyush Mehrotra as an invited speaker.

 http://sc14.supercomputing.org/blog/sc14-announces-new-plenary-focus-importance-supercomputers-society
 - SC14 Announces New Plenary to Focus on the Importance of Supercomputers in Society, Yahoo Finance, October 2, 2014.
 http://finance.yahoo.com/news/sc14-announces-plenary-focus-importance-140000361.html
 - SC14 "HPC Matters" Plenary Presentation, SGI Press Release, October 13, 2014.
 http://www.sgi.com/sc14/plenary.html
 - SC14 Announces New Plenary to Focus on the Importance of Supercomputers in Society, HPCwire, October 16, 2014.
 http://www.hpcwire.com/off-the-wire/sc14-announces-new-plenary-focus-importance-supercomputers-society-2/
- NASA Ames Research Center's 75th Anniversary Open House, October 18, 2014—NAS staff organized, produced, and handled set-up/tear-down of displays showcasing science done at the NAS facility as part of NASA Ames' Open House event. They also interfaced with the general public throughout the day, communicating the division's place at Ames and within NASA as a whole (see slide 8).

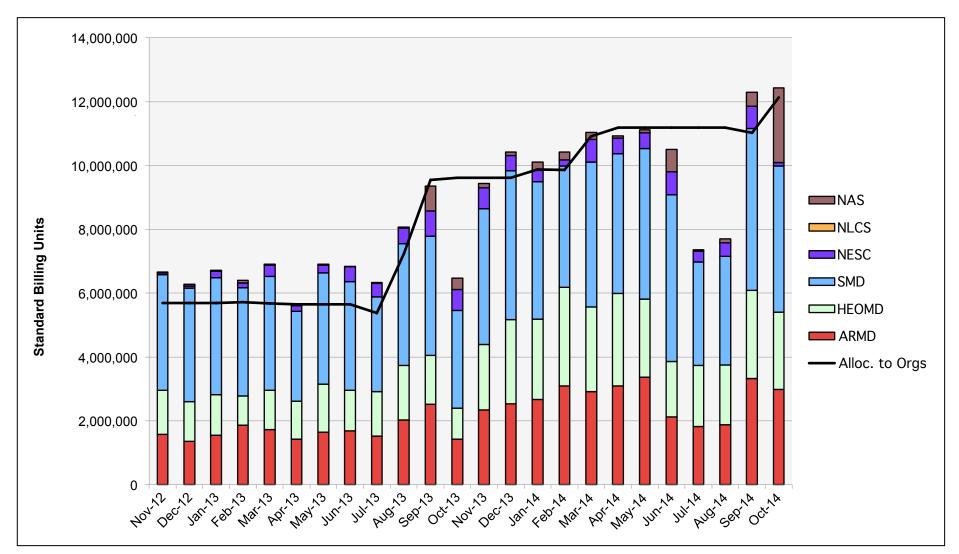
HECC Utilization





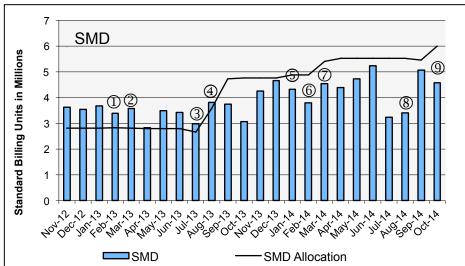
HECC Utilization Normalized to 30-Day Month

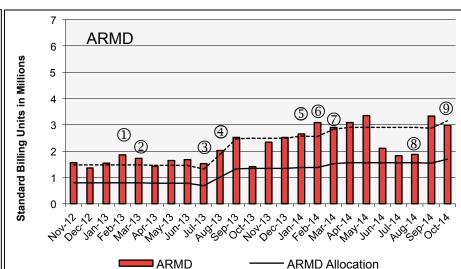


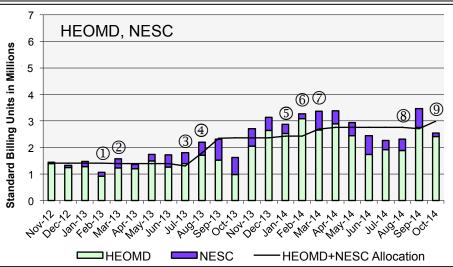


HECC Utilization Normalized to 30-Day Month









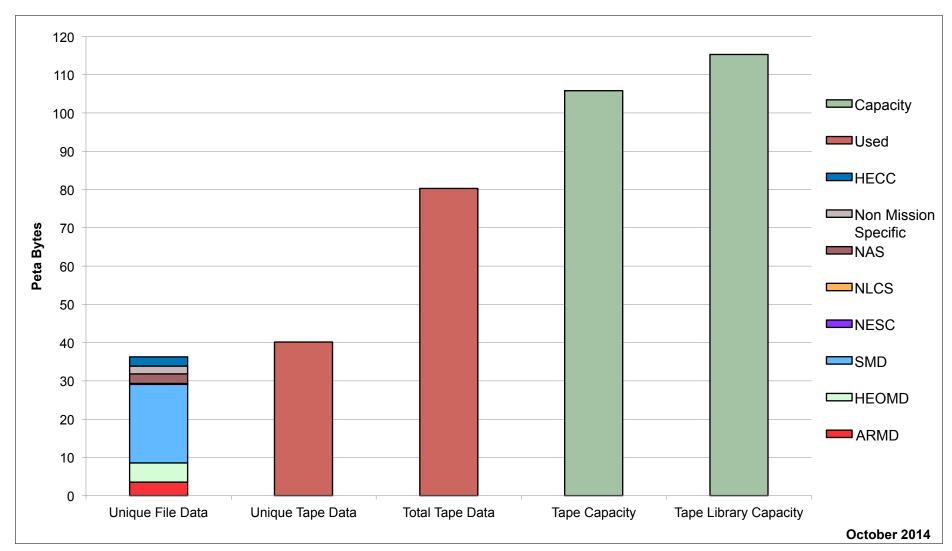
- ① Columbia 21, 23, and 24 retired, Endeavour 2 added
- 2 Columbia 22 retired; Endeavour 1 added
- 3 32 Harpertown Racks retired

Feb.

- ④ 32 Harpertown Racks retired; 46 Ivy Bridge Racks added
- ⑤ 6 Ivy Bridge Racks added; 20 Nehalem, 12 Westmere Racks Retired
- 8 Ivy Bridge Racks added mid-Feb; 8 additional Ivy Bridge Racks late
- 4 Ivy Bridge Racks added mid-March
- 8 6 Westmere Racks added to Merope, Merope Harpertown retired
- 9 10 Nehalem Racks and 2 Westmere Racks added to Merope; 3 Ivy Bridge Racks added mid-Oct; 15 Haswell Racks added in late Oct.

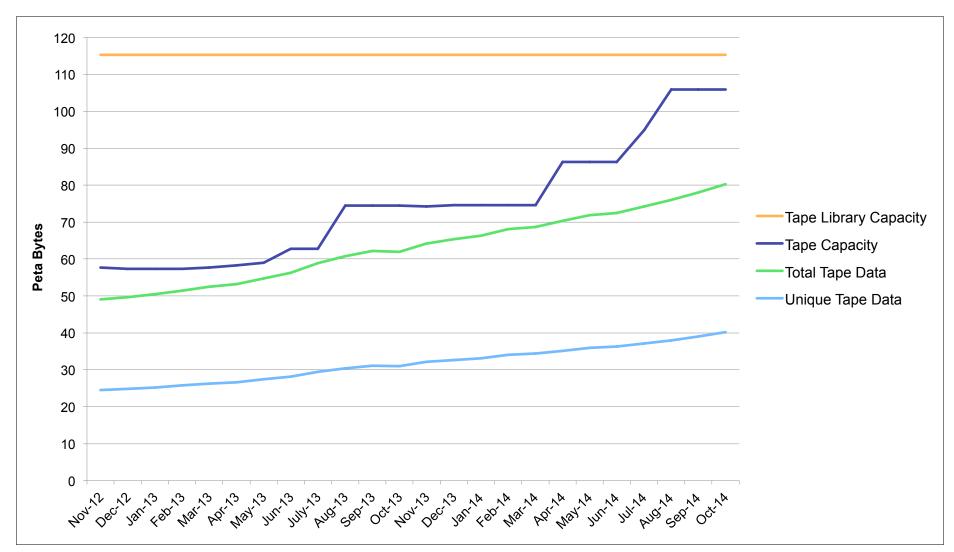
Tape Archive Status





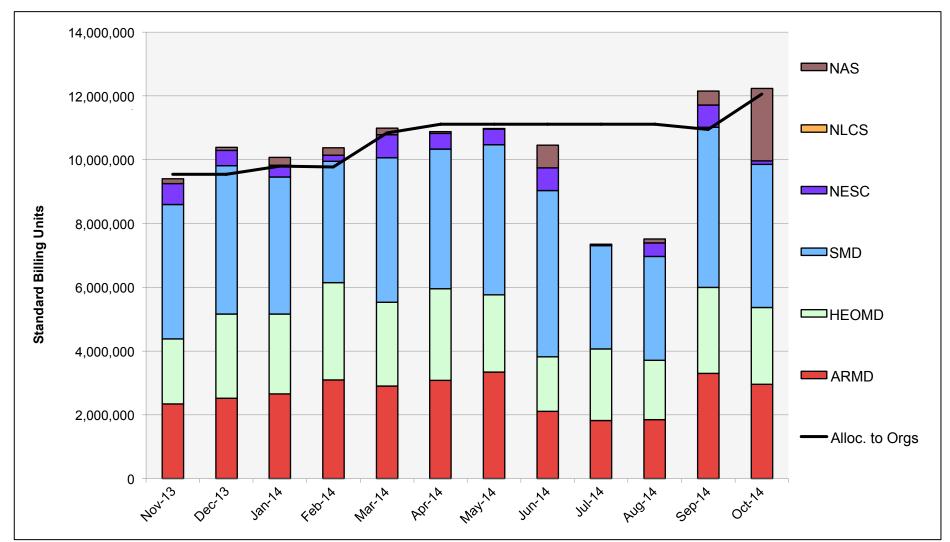
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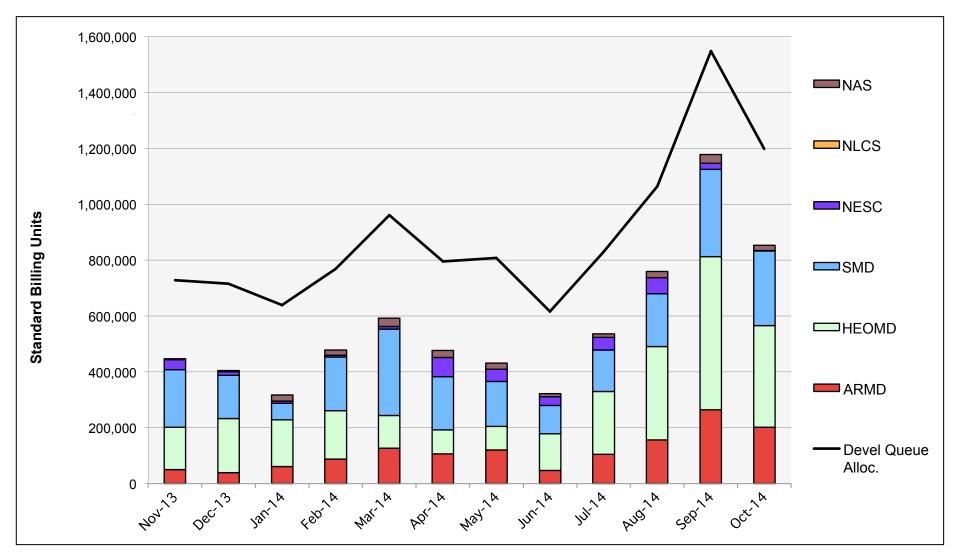
Pleiades: SBUs Reported, Normalized to 30-Day Month





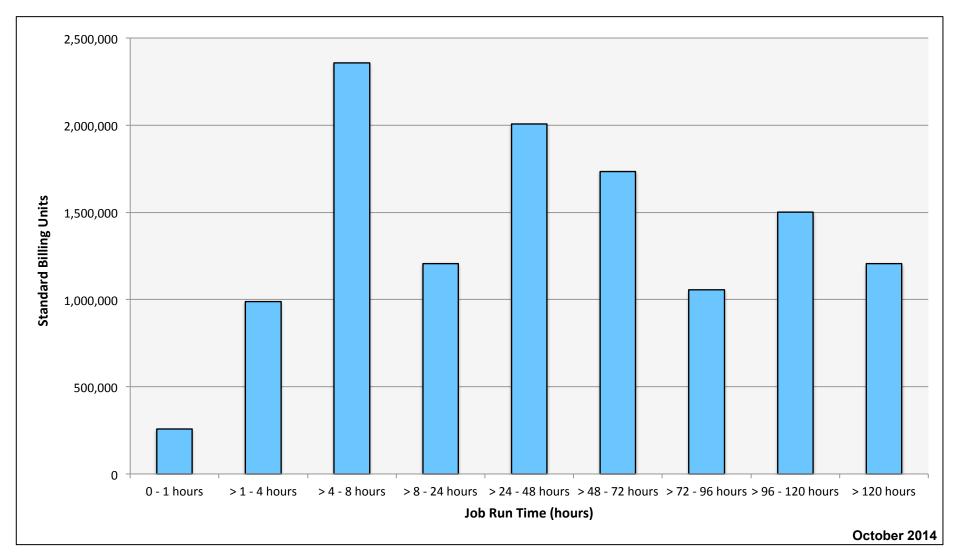
Pleiades: Devel Queue Utilization





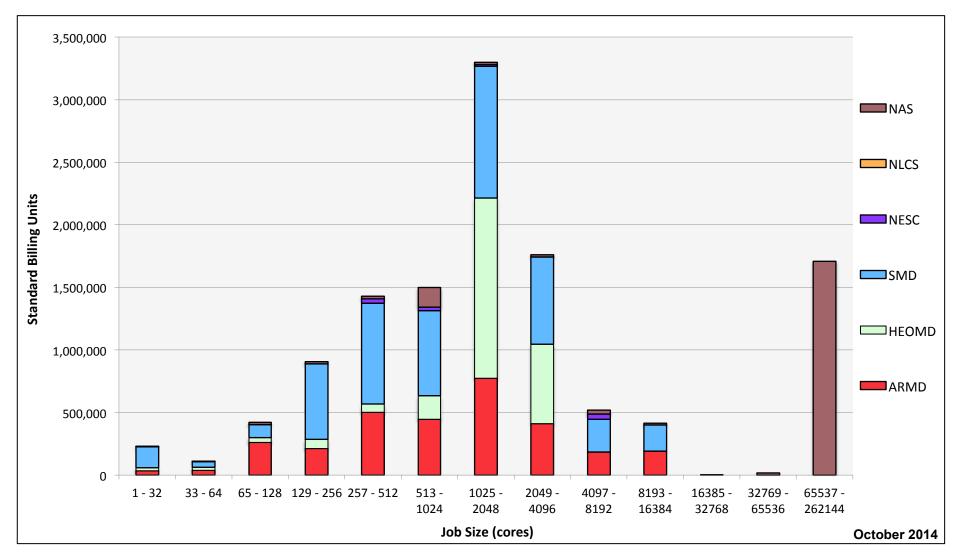
Pleiades: Monthly Utilization by Job Length





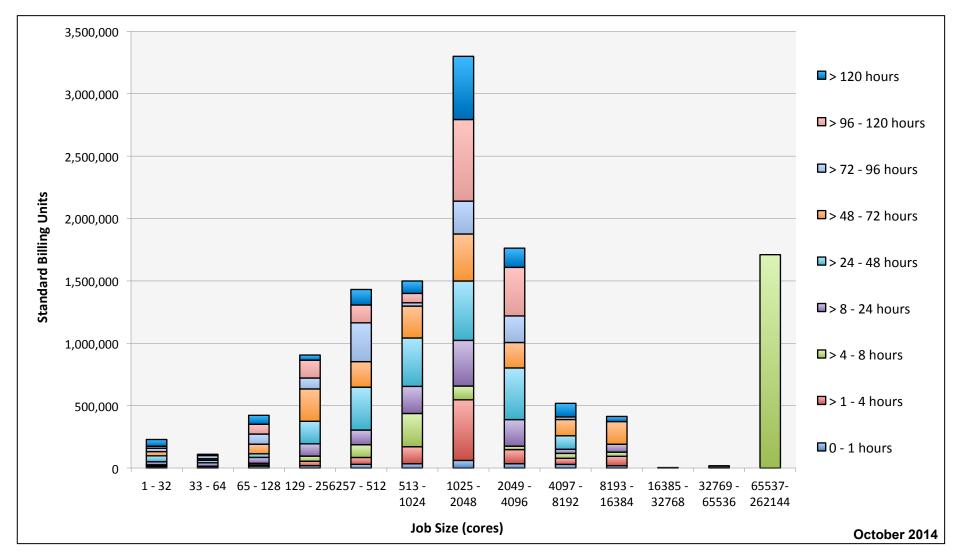
Pleiades: Monthly Utilization by Size and Mission





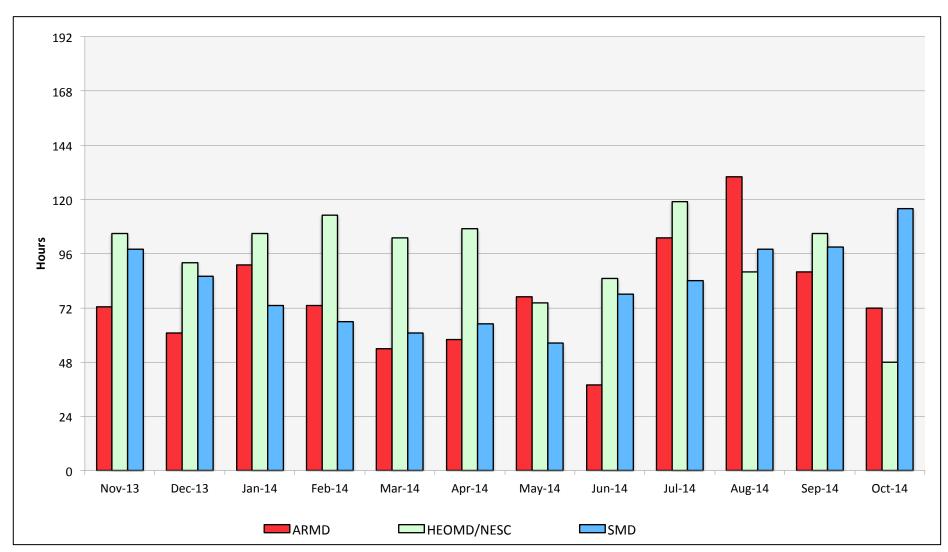
Pleiades: Monthly Utilization by Size and Length





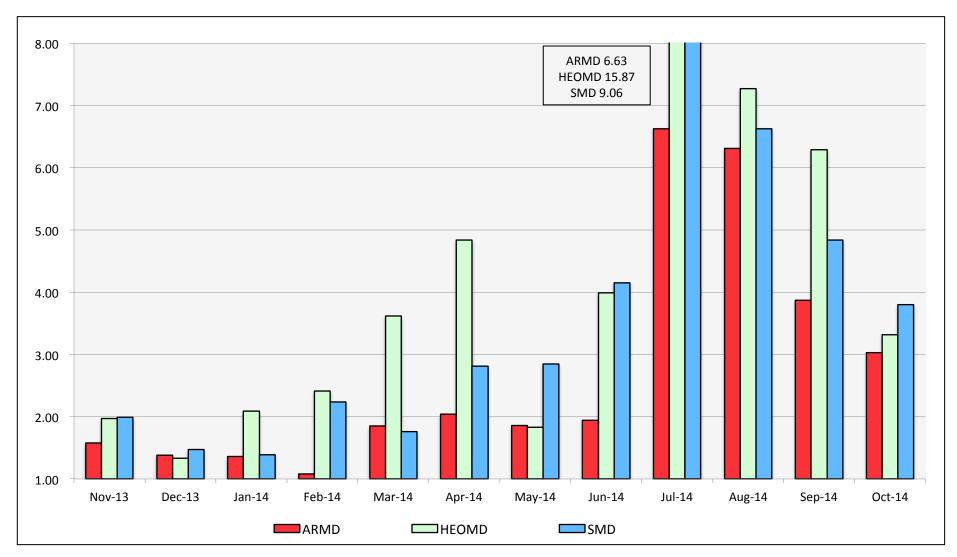
Pleiades: Average Time to Clear All Jobs





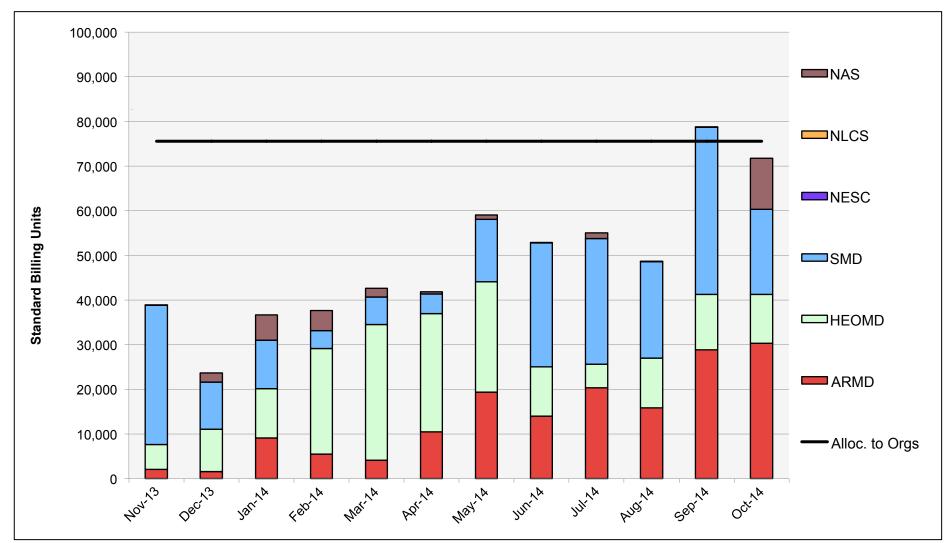
Pleiades: Average Expansion Factor





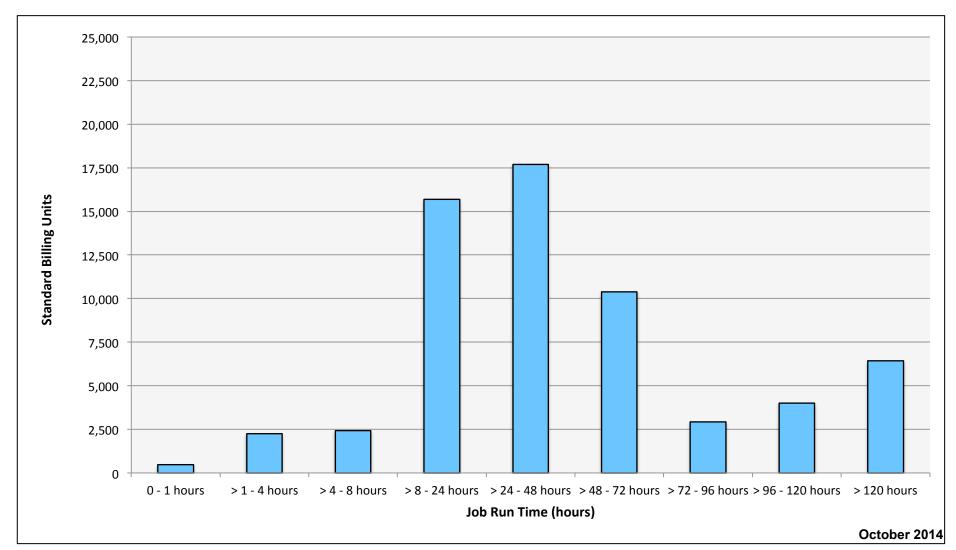
Endeavour: SBUs Reported, Normalized to 30-Day Month





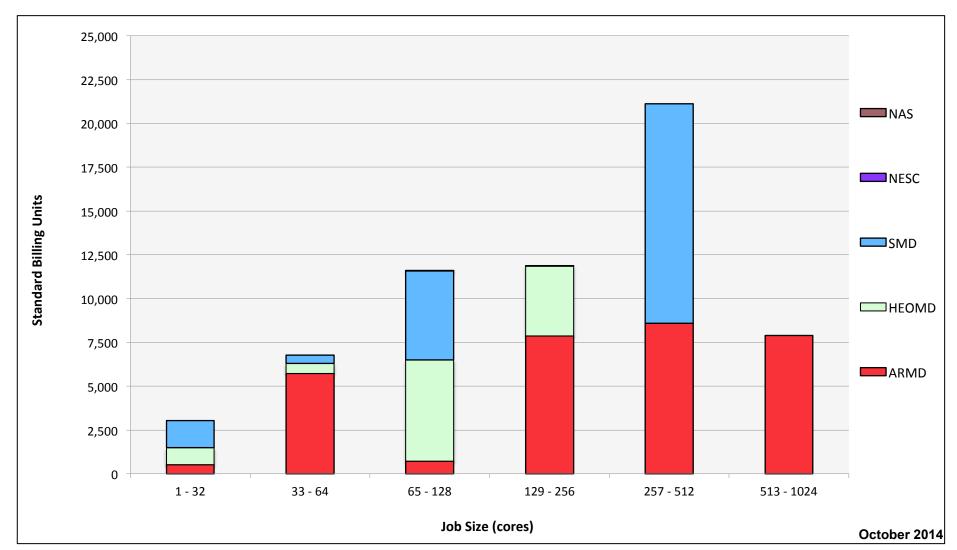
Endeavour: Monthly Utilization by Job Length





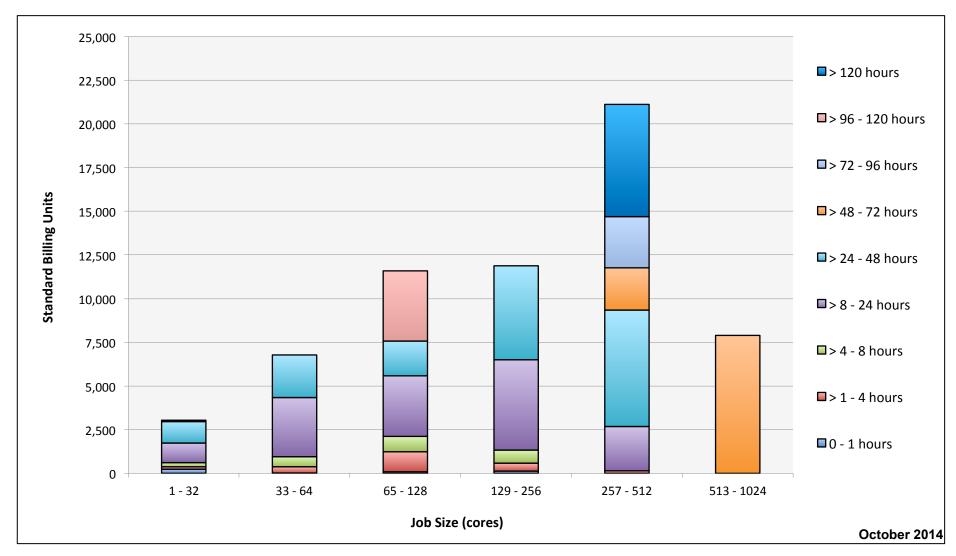
Endeavour: Monthly Utilization by Size and Mission





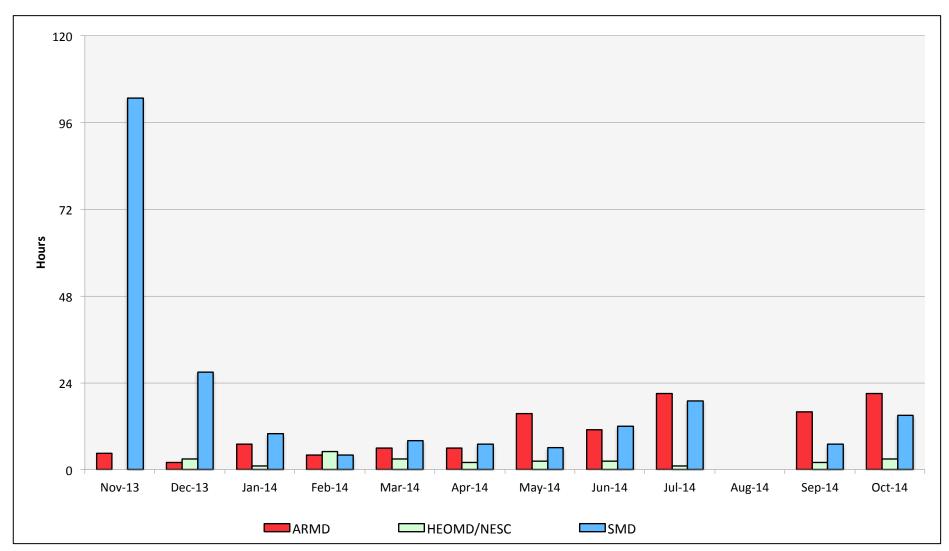
Endeavour: Monthly Utilization by Size and Length





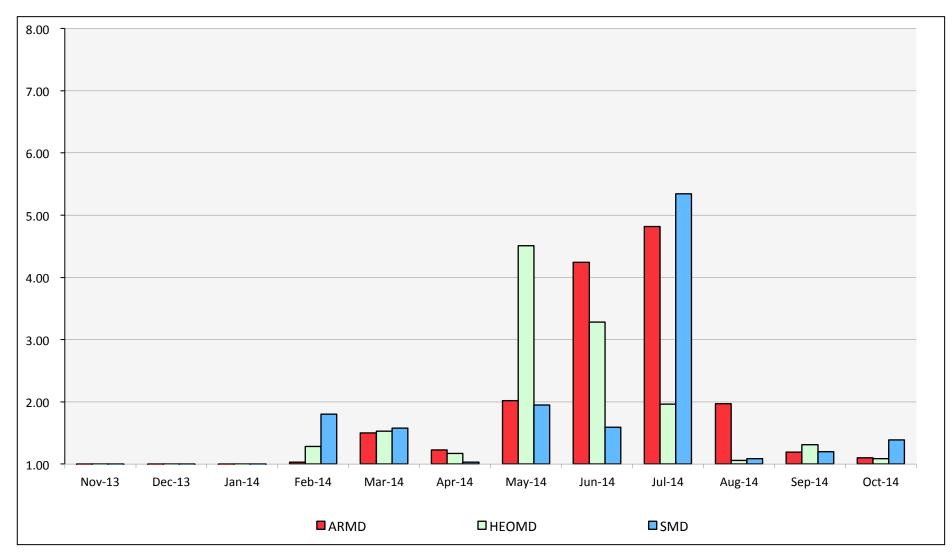
Endeavour: Average Time to Clear All Jobs





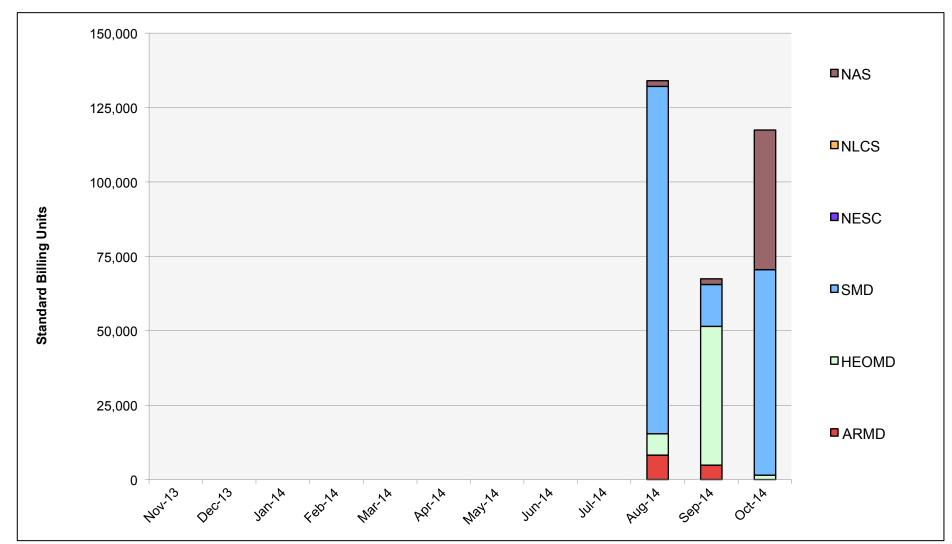
Endeavour: Average Expansion Factor





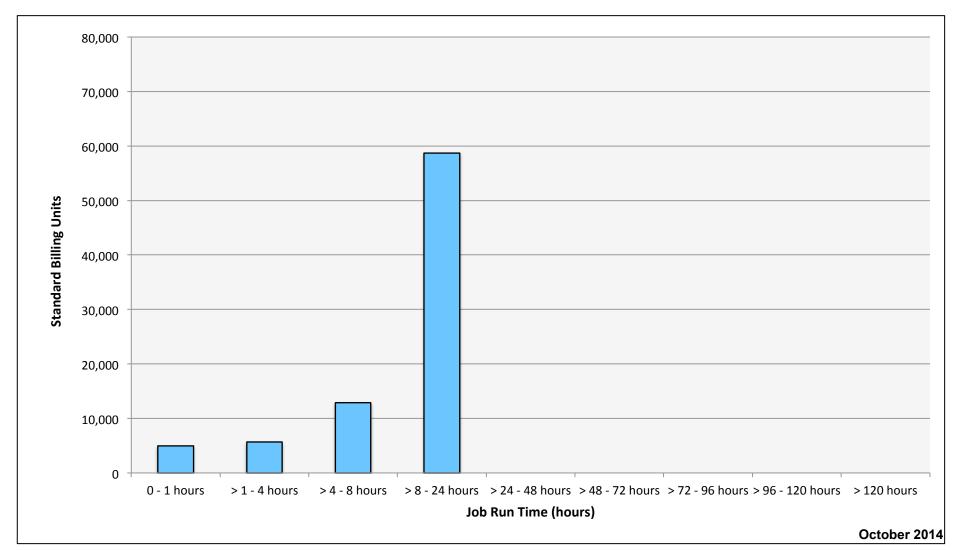
Merope: SBUs Reported, Normalized to 30-Day Month





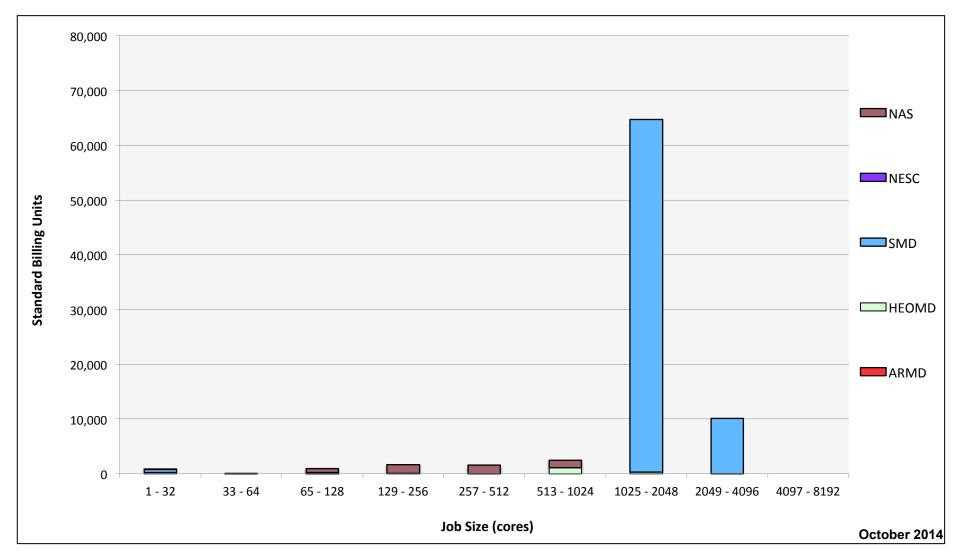
Merope: Monthly Utilization by Job Length





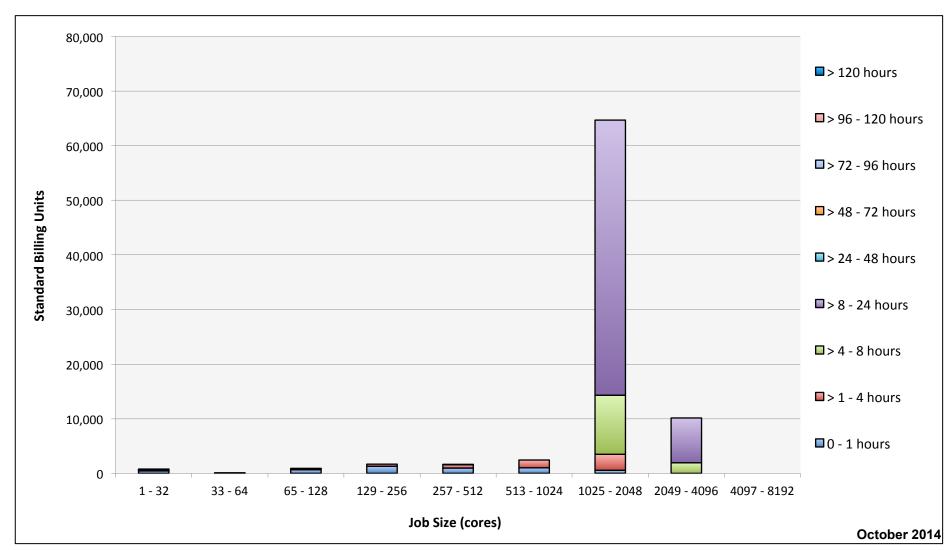
Merope: Monthly Utilization by Size and Mission





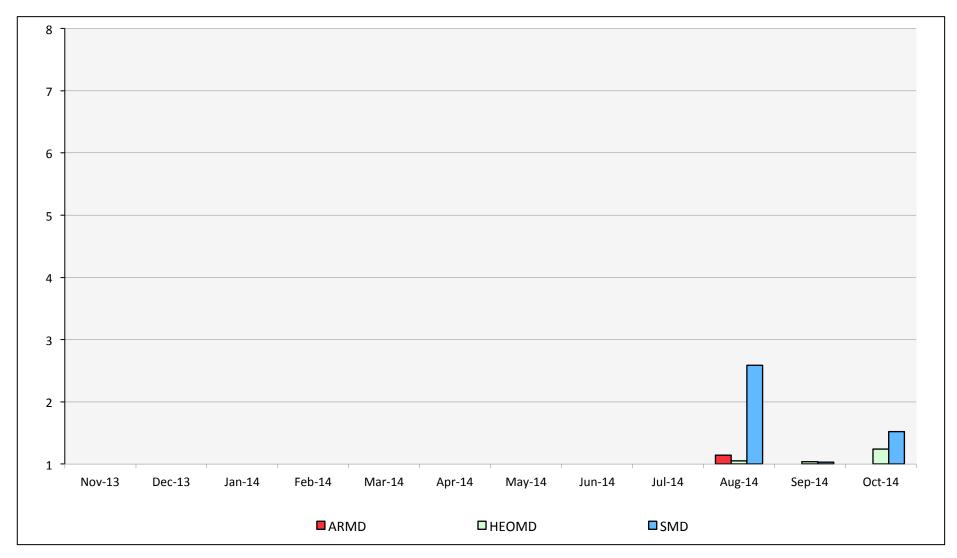
Merope: Monthly Utilization by Size and Length





Merope: Average Expansion Factor





Maia: SBUs Reported, Normalized to 30-Day Month



